U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND – ARMY RESEARCH LABORATORY

Applicants’ Day Workshop for High-Throughput Materials Discovery for Extreme Conditions (HTMDEC)

Chris Haines, Scott Schoenfeld, Debjoy Mallick

CAM, ST-Terminal Ballistics, Deputy CAM

WMRD

29 July 2021

TODAY'S AGENDA

Time		
0900/910	Collaborative Research in WMRD/ARL	J. Zabinski (or alternate VIP)
0920	HTMDEC Overview	C. Haines
1000	Contracting & Legal Overview	R. Moxley
1030	Morning Break – Attendees Can Submit Questions	
1045	Physics of Soldier Protection to Defeat Evolving Threats	C. Hoppel
1115	Science of Additive Manufacturing for Next Generation Munitions	J. Robinette
1145	Long Range Distributed and Cooperative Engagements	F. Fresconi
1215	Hypersonics Materials OV	Victoria Blair
1240	Lunch Break	
1315	Morning Wrap-up, Afternoon Charge & Answer to Submitted Questions	Haines/Mallick
1415	Materials & Manufacturing OV	Bryan Love
1440	Protection Materials OV	Lionel Vargas
1505	Afternoon Break	
1515	Lethality Materials OV	Phil Jannotti
1540	Data Science OV	Chris Rinderspacher
1605	Closing Comments	C. Haines

MOST IMPORTANT SLIDE

The purpose of this workshop is to give potential applicants a chance to learn more about the HTMDEC FOA, ask questions, and hear about technical challenges from potential transition partners. However, at the end of the day: **Nothing we say here today in this workshop will supersede what is in the actual FOA (**posted on Grants.gov). We will do our best to avoid presenting any conflicting information, and answering your questions to the best of our ability, but the FOA will be the **defining document** that the government will follow.

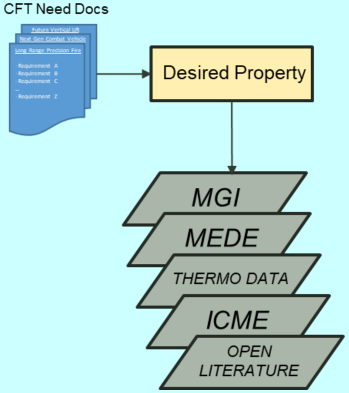
OUTLINE

- BLUF –Vision/Endgame
- HTMDEC Timeline
- Pertinent HTMDEC links (FOA, website)
- What HTMDEC is
- What HTMDEC is <u>not</u>
- New Directions
- Seedlings & Centers
- ARL-Internal HTMDEC efforts
- Technical Thrust Areas
  - Targeted
  - General
- Workforce Development

WHERE ARE WE GOING? ENDGAME

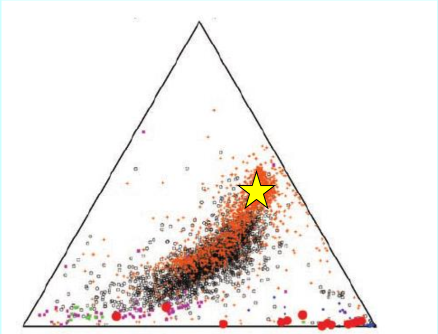
Program Goal: Develop the methodologies, models, algorithms, synthesis & processing techniques, and characterization methods to rapidly accelerate the discovery of novel materials for extreme conditions.

Discover



CFT Defines Operational Requirement

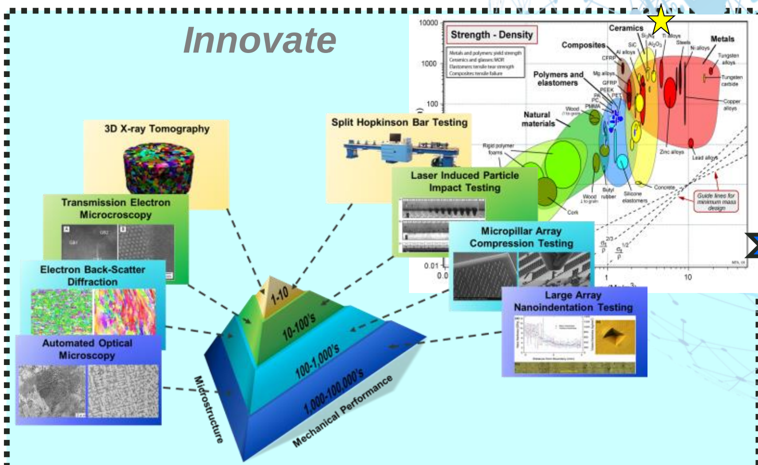
Data Informatics



Notional Phase Diagram

AI/ML driven material selection

Innovate



High Throughput Synthesis & Characterization

Transition

Next Gen Ceramic Armor Protection

Hypersonic Leading Edges

HTMDEC TIMELINE

YOU ARE HERE

Materials Discovery Workshop held virtually	October 2020	✓
FOA Draft to Legal & ACC for Input	Jan 2021	✓
Pre-Solicitation release	June 2021	✓
HTMDEC website goes live	29 June 2021	✓
Final Opportunity release	July 2021	✓
FOA Opportunity Workshop	29 July 2021	
Deadline for Questions on Funding Opportunity	6 August 2021	
Whitepapers Due	31 August 2021	
Invitations for Proposals	October 2021	
Proposals due	1 November 2021	
Seedling Awards	January 2022	

HTMDEC OPPORTUNITY ANNOUNCEMENT

HOME | LEARN GRANTS | SEARCH GRANTS | APPLICANTS | GRANTORS | SYSTEM-TO-SYSTEM | FORMS | CONNECT | SUPPORT

GRANTS.GOV 〉 *Search Grants*

VIEW GRANT OPPORTUNITY

« Back | Link

W911NF-21-S-0013
High-Throughput Materials Discovery for Extreme Conditions (HTMDEC)
Department of Defense
Dept of the Army -- Materiel Command

Apply | Subscribe

SYNOPSIS | VERSION HISTORY | RELATED DOCUMENTS | PACKAGE

Print Synopsis Details

General Information

Document Type: Grants Notice

Funding Opportunity Number: W911NF-21-S-0013

Funding Opportunity Title: High-Throughput Materials Discovery for Extreme Conditions (HTMDEC)

Opportunity Category: Discretionary

Opportunity Category Explanation:

Funding Instrument Type: Cooperative Agreement

Category of Funding Activity: Science and Technology and other Research and Development

Category Explanation:

Expected Number of Awards:

CFDA Number(s): 12.630 -- Basic, Applied, and Advanced Research in Science and Engineering

Cost Sharing or Matching Requirement: No

Version: Synopsis 3

Posted Date: May 14, 2021

Last Updated Date: Jul 15, 2021

Original Closing Date for Applications: This announcement is currently in a pre-release stage. The Government is currently seeking feedback from industry and the university/non-profit community on the contents of the announcement prior to releasing the official Funding Opportunity Announcement. The official announcement is expected to be released in June 2021. Until that announcement is released, the Government will be accepting feedback via email at usarmy.rtp.devcom-arl.mbx.baa3qa@mail.mil.

Current Closing Date for Applications: Nov 01, 2021 This announcement is currently in a pre-release stage. The Government is currently seeking feedback from industry and the university/non-profit community on the contents of the announcement prior to releasing the official Funding Opportunity Announcement. The official announcement is expected to be released in June 2021. Until that announcement is released, the Government will be accepting feedback via email at usarmy.rtp.devcom-arl.mbx.baa3qa@mail.mil.

Archive Date:

Estimated Total Program Funding:

Award Ceiling: $2,500,000

Award Floor: $150,000

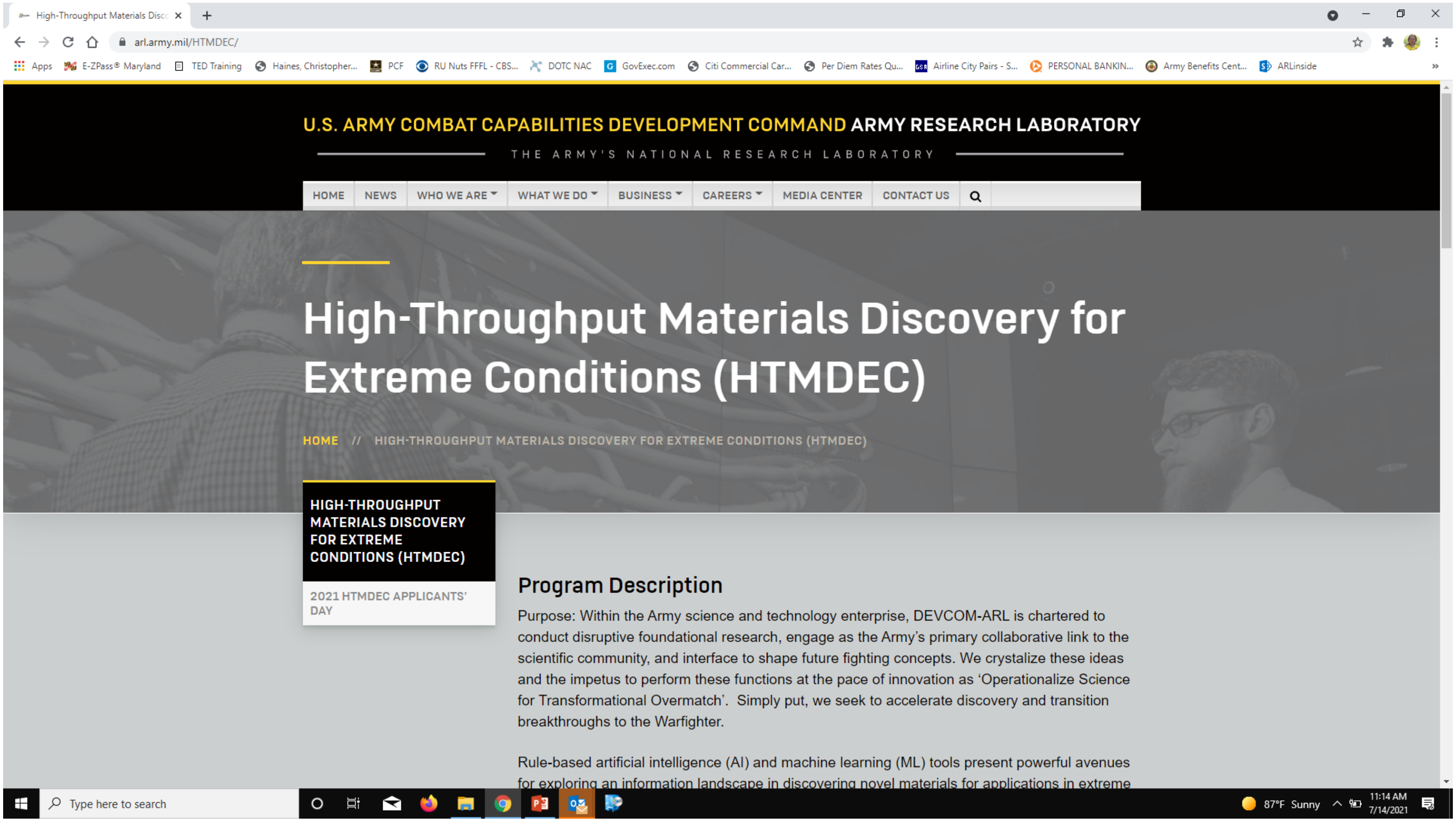
Eligibility

Eligible Applicants: Others (see text field entitled "Additional Information on Eligibility" for clarification)

Additional Information on Eligibility: Eligible applicants under this BAA include institutions of higher education, nonprofitorganizations, and for-profit organizations (i.e. large and small businesses) in the United Statesor its territories. This eligibility criteria applies to all applicants involved in the substantiveefforts of a proposal (e.g., the Recipient).

HTMDEC WEBSITE IS NOW LIVE

https://arl.army.mil/HTMDEC



Special thanks to Jenna Brady and her team for their support

WHAT HTMDEC IS…

The overarching goal of this program is to couple automation and machine learning techniques to material manufacturing and characterization to demonstrate **new materials** that withstand and perform under *extreme conditions*. The program will *develop* the necessary methodologies, models, algorithms, synthesis & processing techniques, and requisite characterization and testing to **rapidly accelerate the discovery of novel materials through data-driven approaches**. As such, it is expected the results of this program will be the above techniques as well as **novel materials** exhibiting *unprecedented properties* at the appropriate scales that have been developed utilizing all of the aforementioned tools which will be provided to DEVCOM-ARL for further analysis and testing.

- New Methodologies
- New Models
- New ML algorithms
- New HT Synthesis & Processing Techniques
- New HT Characterization & Testing Techniques

Next gen materials for extreme conditions, discovered at an *accelerated* pace

WHAT HTMDEC IS NOT…

- A continuation of our previous CRA (Materials for Extreme Dynamic Environments - MEDE) – This is a brand new initiative, with many changes

- A program with a rigid structure for the next 5-10 years – we will be a dynamic program pivoting on the fly as the R&D develops

- ICME 2.0 – While ICME will likely play a role in any HT program, the focus is not to optimize the ICME methodology, but to extend HT processes through the entire lifecycle of materials development

- A program looking to fine tune, tweak, and/or recycle existing ML algorithms and models that have been developed for big data – Materials as a whole is a relatively sparse data set, materials for extreme conditions even more sparse

- A program with the intent of **only** developing new “tools” (algorithms, models, synthesis and characterization techniques, characterization techniques – **novel materials** using these tools is essential to the success of this program

HTMDEC - NEW DIRECTIONS

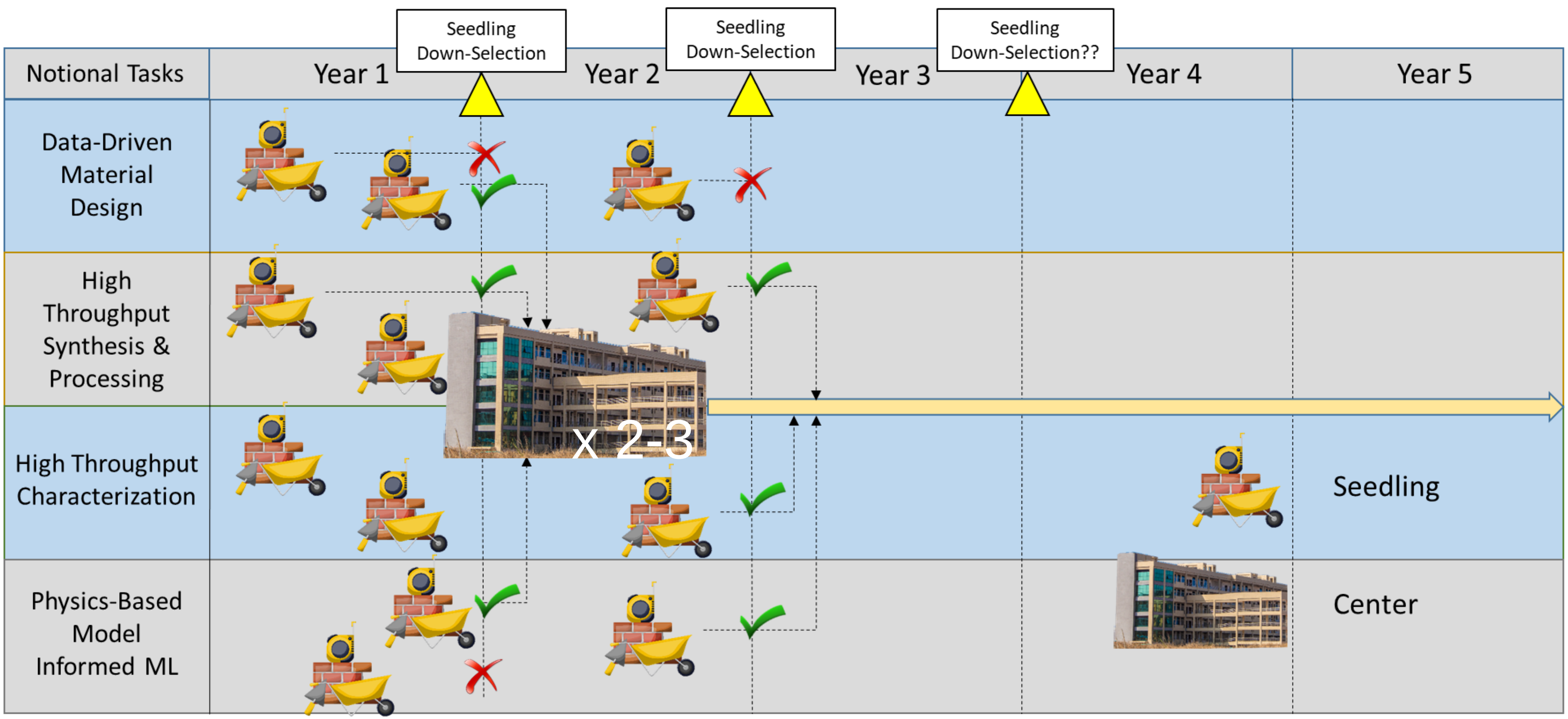
- **Previous CRAs**
  - Advertised via Broad Agency Announcement (BAA)
  - Large ‘Center’ from the onset of program
  - One major, multi-year contract with multiple co-PIs (MURI model)
  - Limited flexibility for Government to run an agile program

- **HTMDEC**
  - Advertised via Funding Opportunity Announcement (FOA)
  - Awarded via multiple Cooperative Agreements (CAs)
  - Program initiates with numerous ‘Seedlings’, down-select to a few ‘Centers’ (closer to DARPA model)
  - Seedlings are of limited duration. They are expected to matriculate into part of a center (success) or terminate.
  - Centers + Seedlings in out-years, successful seedlings can be rolled into Centers
  - All participants are expected to participate in collaboration events; this will be one of the mechanisms for interaction between seeds, interactions with the WMR workforce and development of centers.
  - Encourages **workforce development** by offering Fellowships for graduate students who are US Citizens (in Centers)

SEEDLING & CENTER CONCEPT

Seedling – single year, narrowly focused (1 or 2 thrust areas) effort

Center – multiple year effort, comprehensive effort (must address all 4 thrust areas).



ARL-INTERNAL HTMDEC PROJECTS

In order to promote fruitful collaborations between ARL and University partners, we have decided to run an internal proposal process in conjunction with the extramural process. The white paper/full proposal process, as well as program reviews, will run in parallel to assure selection of internal projects with strong alignment with the Centers.

It is expected that PIs chosen for internal projects will foster concrete collaborations with University partners within the HTMDEC Centers and essentially become “champions” of this research at ARL. This will work to maximize the likelihood of technology adoption and transition over time. Yearly program reviews will present an optimal opportunity to build these partnerships.

For Year 1, since no Centers have been chosen, we will look to fund projects which look to rapidly develop technologies that augment ARL’s HT capabilities.

SOME CLARITY ON SEEDLINGS & CENTERS

There were many comments during the pre-solicitation phase of the FOA in this area, so clearly this area needs some clarification – some of which was integrated into the FINAL FOA language

- Why Seedlings? Why not allow Centers in Year 1? A few reasons:
  - As previously mentioned, we want to be an agile program. Moving out with a couple anchor programs in Year 1 relinquishes that agility.
  - This program is going to be challenging. It requires materials scientists working with data scientists, experimentalists working with theoretical shock physicists, etc. – this needs thoughtful planning.

- Can Seedlings be multi-University? Yes, 100%...however, each co-PI will obviously have limited funds during this year

- Can prospective Center co-PIs each seek their own Seedlings and then coalesce into a Center? 100%, and this is one of the intente of this structure. We hope to see successful seedlings merged into Centers, not only in Year 2…but continuing in out-years

- How many Seedlings/Centers per year? We anticipate ~ **10-12** Seedlings in Year 1, and **2-3** Centers plus a **few** Seedlings in out-years

PROGRAM THRUST AREAS

There are two (2) FY22-specific thrust areas that will only be advertised in Year 1 of the FOA. The intent is to allow for effective teaming, program development, establishing a workflow (2022-1) and demonstration of a data handling & management platform that will be utilized throughout the program (2022-2).

FY2022-1 - **Program & Workflow Development**
FY2022-2 – **Data Handling & Management**

1. **Data-driven Material Design** - all aspects of the material design phase in the material development cycle which are accelerated through the integration of computational methods.
2. **High-Throughput Synthesis & Processing** – both modifying existing synthesis & processing methods to accommodate for high-throughput, as well as developing novel techniques.
3. **High-Throughput Characterization** – implementation of automation, as well as development of surrogate tests to mimic high-strain techniques which are not amenable to automation.
4. **ML-augmented Physics-Based Models** – integration of physics-based models with machine learning is poised to be a tipping point in materials science. To date, nearly all ML algorithms have been developed for big data (e.g. image recognition). We must discontinue ‘repurposing’ these algorithms and develop ML algorithms specifically designed for materials discovery, and informed by physics.

DATA-DRIVEN MATERIALS DESIGN

Key Challenges:

• The integration of ML into methodologies like ICME, Materials-by-Design, HT Materials Science rely on large, accurate data sets, but **data in materials science is sparse** in comparison with conventional big data that ML algorithms have been typically designed for

• Data mining/informatics for accelerating materials discovery **better suited for conventional materials** systems (common alloys, traditional ceramics, etc.) than for more exotic materials (HEAs, ultra high temperature ceramics, etc.)

• Plethora of issues with data curation: **data veracity**, **integration of experimental and computational data**, **metadata tagging**, **standardization**, and disparity between industry and academia efforts.

• Data for Army relevant applications is not only sparse, but often **classified** in the realm of extreme conditions (ballistic test data, hypersonic operational parameters, etc.)

HT SYNTHESIS & PROCESSING

Key Challenges:

• HT synthesis of **thin films** has been demonstrated; progress on HT synthesis of **bulk materials** is lagging; microstructure is likely to be highly dependent on particular processing method and variables.

• Successful examples of HT synthesis of metals (e.g., high-entropy alloys) and some polymers are far more common than ceramics or composites; methodologies are **more mature in these classes** of material.

• Most synthesis and processing techniques lack **in situ** diagnostics and/or characterization; additive manufacturing may lead here.

• Processing is a major challenge. In contrast to synthesis, processing maps are ill-explored and offer simple guidance, if any. There is no straightforward or unified way to represent/encode processing history. Processing techniques vary widely and are sometimes proprietary, based on industrial standards, especially in ceramics. **Process models are often very basic** (e.g., master sintering curves in ceramics). Processing approaches are often in large serial machines (or specific industrial equipment) and require handoff from the synthesis platform.

• Length-scale and **correlation across scales** in bulk materials will be highly challenging:

- o Small samples may not contain defects that dominate behavior of bulk material.
- o Mechanisms can change across scales (e.g., deformation modes and failure).
- o Sensitivity at-scale may depend on application (blast vs. hypervelocity, for example).
- o Optimization may require at-scale alignment between synthesis/processing and characterization/testing plan.

• HT leads to higher **uncertainty**. There are tradeoffs between speed and accuracy. We must account for human factor (operator biases). Sparse but information-rich experiments are common for lab-scale dynamic experiments.

HT CHARACTERIZATION & TESTING

Key Challenges:

• Lack of **surrogate measurements** that correlate to high-strain rates. Current state of the art: nano-indentation, Raman, gas gun, cylinder expansion, laser shock, and micro-Kolsky. There is also a dire need for **in situ** methods to capture high-rate data.

• Clearly define a **hierarchy of characterization/testing** such that the high-strain-rate tests are only on a handful of elite candidate materials.

• **Rate-limiting steps** need to be identified and targeted during development of workflow.

• There exists a human bottleneck in nearly every characterization technique. Need for **automated and/or autonomous** characterization systems with controlled data quality and understandable pedigree. Areas ripe for development include the following: automated microscopy to assess morphology, Raman, Fourier-transform infrared, micro-ballistics, nano-indentation, and Kolsky bar.

• Lack of **uncertainty qualification** across the entire process, as well as across scales.

• Leverage processing capabilities unique to Army in-house programs; these are specialized to Army requirements and ready to partner with industry.

ML-AUGMENTED PHYSICS-BASED MODELS

Key Challenges:

• ML tools for materials science are only just emerging; they currently **lack connection to highly specialized physics-based models**. Physics-based techniques for ICME are still under development. Scale bridging — **quantification of nonlinear bulk properties** based on collective behavior of small defects— remains challenging. Direct incorporation of ICME tools within an ML framework could be computationally overwhelming.

• ML-enhanced models for **transient phenomenon** such as failure are inherently at a disadvantage because the phenomena **time/length scale** is much smaller than the material/structure scale.

• Current models are not user-friendly; **more flexibility** is required and models need to account for failure anywhere in the process. To be compatible with ML processes, **models need to be reconfigurable** as data quality and quantity improve.

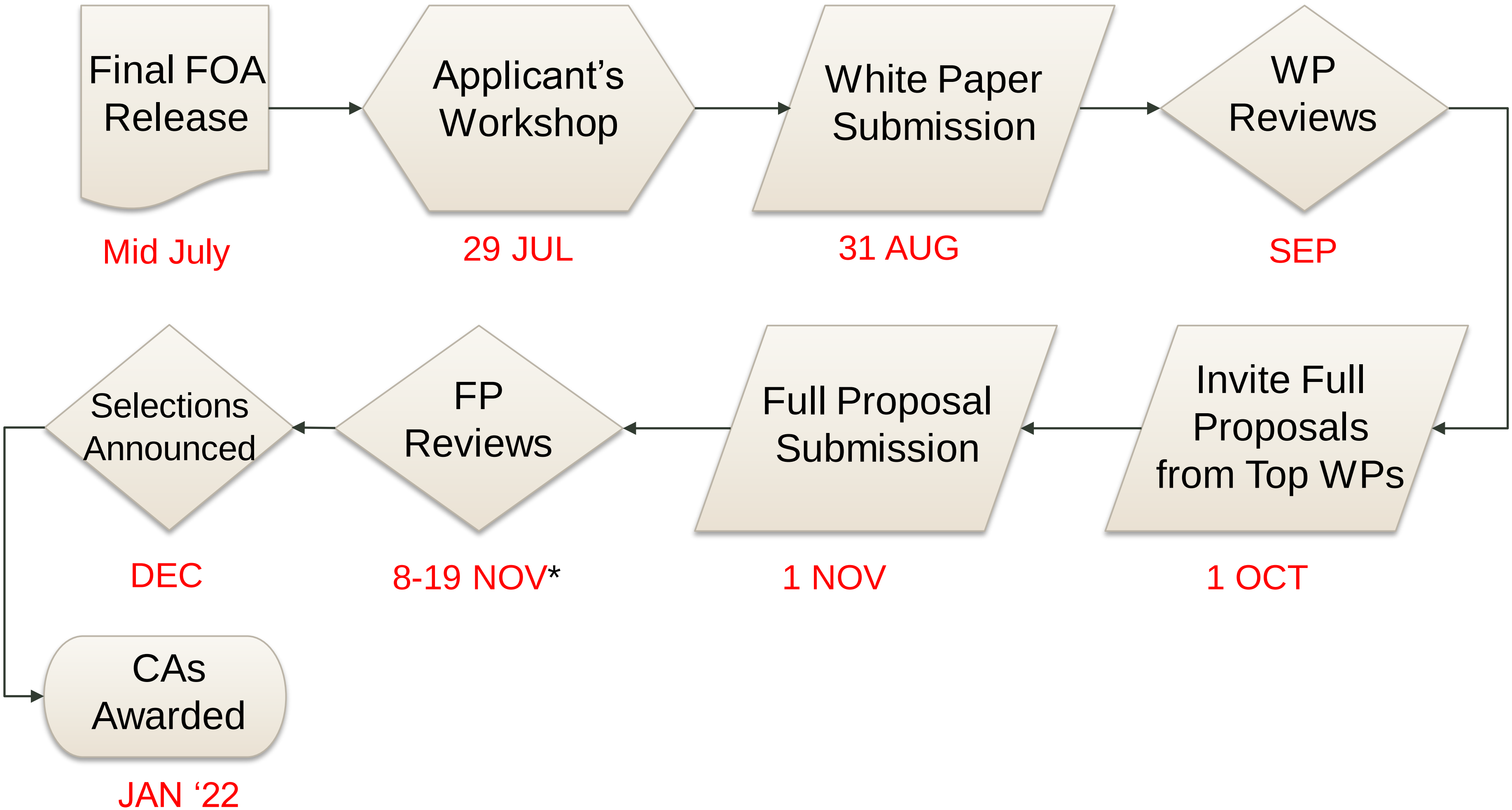
• Data quantity to **train ML methods**. Quantity of high-rate characterization is small. Experiments requires care and precision; currently a low-volume activity.

• Data formats are **nonstandard and non-centralized**. Human inertia is high.

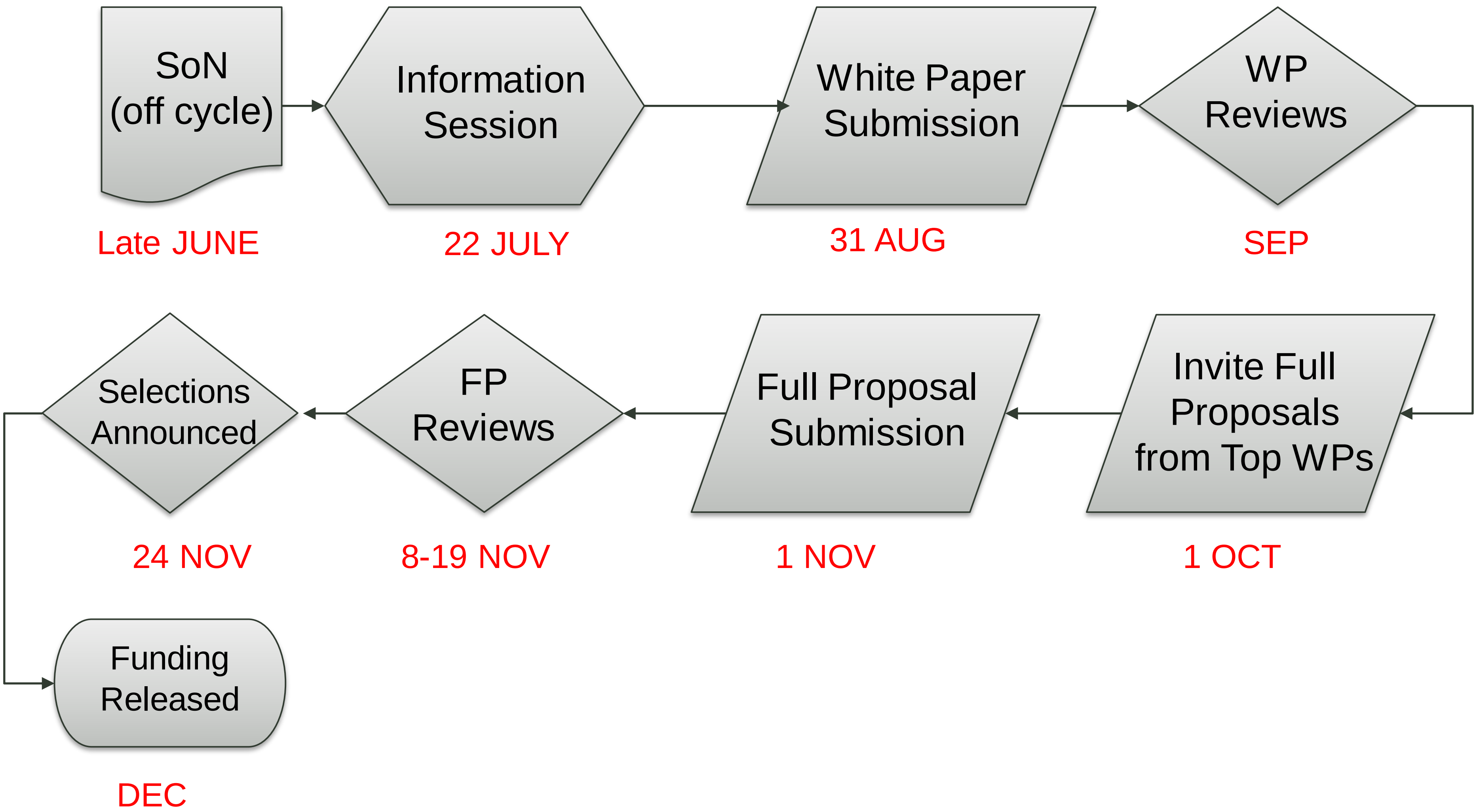
• **Uncertainty** pervades both bulk materials and final application; **quantification** is difficult.

• Some ML cannot be easily explained, and can even be difficult to interpret. Information security surrounding ballistic applications may impede open across-the-enterprise transparency and only exasperate these issues.

EXTRAMURAL PROPOSAL PROCESS



PROPOSED INTERNAL PROPOSAL PROCESS



WORKFORCE DEVELOPMENT

- This CRA plans on putting a major focus on workforce development
- US Army wants the best & brightest from their University collaborators, and Universities want their students landing rewarding jobs, so this is a win-win
- We will be incentivizing using US graduate students in the HTMDEC program by providing program “fellowships” to Centers in the form of “plus up” funding for Professors who utilize US graduate students
- The intent of these fellowships is to maximize the likelihood of bringing much needed talent into ARL that will be savvy in both material science and data science (ML/AI), clearly the future of materials science
- Actual fellowship amounts and the details are still being determined

MOST IMPORTANT SLIDE (AGAIN!)

The purpose of this workshop was to give potential applicants a chance to learn more about the HTMDEC FOA, ask questions, and hear about technical challenges from potential transition partners. However, at the end of the day, n**othing we say here today in this workshop will supersede what is in the actual FOA (**posted on Grants.gov). We will do our best to avoid presenting any conflicting information, and answering your questions to the best of our ability, but the FOA will be the **defining document** that the government will follow.